Small Business Innovation Research/Small Business Tech Transfer

Computational Tool for Kinetic Modeling of Non-Equilibrium Multiphase Flows in Ablation, Phase I

Completed Technology Project (2009 - 2009)

Project Introduction

Development of highly accurate tools to predict aerothermal environments and associated effects on vehicles is needed to enable advanced spacecraft for future NASA missions. At heating rates encountered during hypersonic reentry, the surface is ablating and the interaction of ablation products blowing into the boundary layer induces new interactions (chemical reactions, radiation absorption) that have strong impacts on surface heating rates and integrated heat loads. One important effect of the reentry phenomenon is the interaction of the ablated debris with the atmospheric gas molecules and vehicle surface. Even though the ablated debris may include particles ranging from the micron-scale down to the molecular scale, the available models of ablation flows only incorporate ablated molecules and neglect molecular clusters. In this project, we will develop computationally-efficient methodology for coarse-grained yet accurate characterization of cluster reactions with the aid of molecular dynamics (MD) simulations and parametric chemistry models. The resultant product will be a software module which will provide the cluster reaction characterization for the given interaction potential. This module will be compatible with existent NASA codes applicable for continuous or rarefied gas regimes. Another software model will perform MD simulations of energetic gas flow surface interaction.

Anticipated Benefits

Modeling of aerodynamic ablation, including the ablation debris flow interactions is of interest to DOD. In particular, ablators are used in ballistic missiles and accurate modeling of ablation process is required for optimization of missile design. Another important aspect is the prediction of optical signatures of ballistic missiles and other objects. Since clusters strongly affect the flow in the vicinity of a hypersonic projectile, the luminous species such as CN will be affected as well. The more commercially-oriented applications are intended for the industry working in the fields of materials fabrication, nano-technology, space technology, MEMS and NEMS. The principal advantage of our product to be developed over Phases I and II is unprecedented physical accuracy of modeling the processes of cluster formation and evolution in non-equilibrium gas environment. To the best of our knowledge, no product of such capability is currently available in the market and we expect high interest and demand. The implementation of our product will allow the user to accurately model physical processes in such technological segments as pulsed laser deposition of thin films, cluster deposition, obtaining of size-selected clusters, micro-thrusters and other space application. This modeling will impart a better understanding of the underlying physics and provide a basis for technology improvement. The principal advantage of our product to be developed over Phases I and II is unprecedented physical accuracy of modeling the processes of particulate interactions within non-equilibrium gas environment. The proposed research will provide information on clustering in terms of spatial distributions of cluster size, kinetic and internal energies, and

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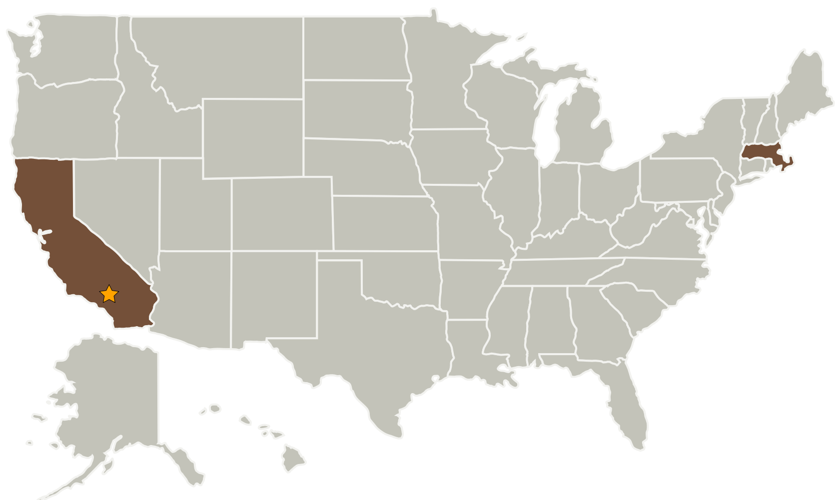
on the dependence of these distributions on the initial conditions and the reaction types. The product to be developed during Phases I and II is directly applicable to the NASA efforts in computational modeling of the entry and reentry space vehicles under the Aeronautics Research Directorate. It is also applicable to the needs of space exploration program under the Exploration Systems Directorate.

Primary U.S. Work Locations and Key Partners



Organizations Performing Work	Role	Type	Location
★Armstrong Flight Research Center(AFRC)	Lead Organization	NASA Center	Edwards, California
Luminad Technologies	Supporting Organization	Industry	Sharon, Massachusetts

Primary U.S. Work Locations	
California	Massachusetts

Organizational Responsibility

Responsible Mission Directorate:

Space Technology Mission Directorate (STMD)

Lead Center / Facility:

Armstrong Flight Research Center (AFRC)

Responsible Program:

Small Business Innovation Research/Small Business Tech Transfer

Project Management

Program Director:

Jason L Kessler

Program Manager:

Carlos Torrez

Project Manager:

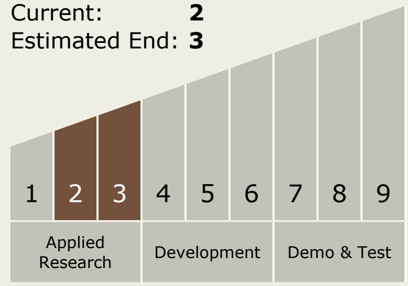
Stephen L Woodruff

Principal Investigator:

Michael Zeifman

Technology Maturity (TRL)

Start: **2**
Current: **2**
Estimated End: **3**



Technology Areas

Primary:

- TX09 Entry, Descent, and Landing
  └ TX09.4 Vehicle Systems
    └ TX09.4.5 Modeling and Simulation for EDL